

X-Ray Soft Mode Intensity for KTaO_3

Lattice constant: $a=4.01 \text{ \AA}$

Atomic Number: $b(\text{K})=19$

$b(\text{Ta})=73$

$b(\text{O})=8$

Mass: $M_{\text{K}}=39$

$M_{\text{Ta}}=181$

$M_{\text{O}}=16$

Atomic displacement (consider only S1 and S2 mode):

$$u_{\text{K}} = -S(M_{\text{Ta}}+3M_{\text{O}})/M_{\text{K}}$$

$$u_{\text{Ta}} = -3M_{\text{O}}/M_{\text{Ta}} + S$$

$$u_{01}=u_{02}=u_{03}=1+S$$

where $S=S2/S1$

The calculated inelastic intensities of KTaO_3 for an arbitrary normalization factor are listed in the table at a parameter $S=0$ and also are plotted in the Figure as a function of the parameter S .

(h k l)	$\alpha F_{inel} ^2 (\text{Cal})$
2 0 0	11
3 0 0	142
1 1 0	183
3 1 0	734

